Scanning the critical fluctuations – application to the phenomenology of the two-dimensional XY-model –

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We show how applying field conjugated to the order parameter, may act as a very precise probe to explore the probability distribution function of the order parameter. Using this 'magnetic-field scanning' on large-scale numerical simulations of the critical 2D XY-model, we are able to discard the conjectured double-exponential form of the large-magnetization asymptote.

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Introduction. − Derivation of the complete equation of state of a many-body system is generally a formidable task. When the system may appear under various phases at the thermodynamic equilibrium, this problem requires knowledge of the exact probability distribution function (PDF) of its order parameter. Despite a number of attempts, just a few instances are available [1]. Even the exact PDF for the 2D Ising model is still unknown.

Within this context, the critical point is very particular, since the universality concept tells us that only a limited information is needed to obtain the complete leading critical behavior. For instance, general arguments give precisely the tail of the critical PDF, $P(m)$, for the large values of the order parameter, m, namely [2]:

$$P(m) \sim e^{-cm^{\delta+1}} , \tag{1}$$

with c a positive constant and δ the magnetic field critical exponent, or the distribution of the zeros of the Ising partition function in the complex magnetic field [3] (such a partition function is Fourier transform of the PDF).

In the present work, we explain how the real magnetic field can be generally used as a very accurate probe to scan quantitatively the zero-field PDF tail, exemplifying the method with the critical 2D XY-model. By the way, we will see that the popular double-exponential approximation of the PDF for this system cannot be correct, and we provide alternative approximation which is consistent with the critical behavior. Consequently, our results discard possible fundamental connexion between this magnetic model and the field of extremal-values statistics.

Former approximation of the magnetization PDF for the critical 2D XY-model. − In a series of recent papers [4, 5, 6, 7], it was argued that the PDF $P(m)$ of the magnetization m of the 2D XY-model at the Berezinskii-Kosterlitz-Thouless (BKT) critical temperature, could be approximated by the generalized Gumbel form:

$$P(m) \propto \exp\left(b_\sigma z_\sigma - \lambda_\sigma e^{a_\sigma z_\sigma}\right) , \tag{2}$$

where the reduced magnetization: $z_\sigma = (m - \langle m\rangle)/\sigma$ is used. From low-temperature spin-wave theory and direct numerical simulations, one obtains [5]:

$$a_\sigma \approx 1.105 \;\; ; \;\; b_\sigma \approx 1.74 \;\; ; \;\; \lambda_\sigma \approx 0.69 \;\; . \tag{3}$$

It was regularly noticed [5] that the form (2) *cannot* be the exact solution of the corresponding statistical problem, even if a number of analytical arguments as well as numerical simulations show convincingly that this trial function is indeed close to the exact solution. Moreover, Eq.(2) is appealing, as it suggests connexion between the critical 2D XY-model and the statistics of extreme variables [8]. Therefore, the question of a possible bridge between these two active fields of statistical physics should be examined precisely. On the other hand, Eq.(2) is inconsistent with the general behavior (1), since $\delta = 15$ for the 2D XY-model. The question to know whether relation (1) is true or wrong for this system, is then fundamentally important. We will examine hereafter these two questions.

Two alternative hypothesis. − We consider the 2D XY-model [9] on a square lattice of size $L \times L$ with periodic boundary conditions. The $N = L^2$ classical spins are confined in the x-y lattice plane, and they interact according to the Hamiltonian: $H = -J\sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$, where $J > 0$ is the ferromagnetic coupling constant and the sum runs over all nearest-neighbor pairs of spins. Eventual critical features are characterized by the singular behavior of the scalar magnetization per site: $m \equiv \frac{1}{N}\sqrt{\left(\sum_i \mathbf{S}_i\right)^2}$, which is a non-negative real number. We define also the instantaneous magnetization direction as the angle ψ such that: $\sum_i S_i^x = mN\cos\psi$ and $\sum_i S_i^y = mN\sin\psi$.

There is a continuous line of critical points for any temperature below the critical BKT temperature T_{BKT}

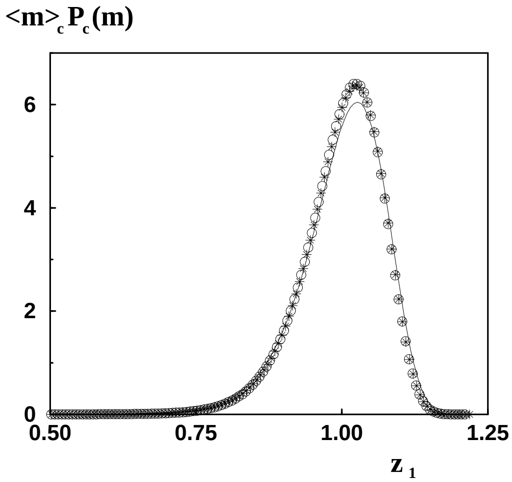

FIG. 1: PDF of the magnetization for the 2D XY-model at the critical temperature T_{BKT}, plotted in the first-scaling form (4). The scaling law is confirmed for $L = 64$ (stars) and $L = 128$ (circles), while the $L = 16$ (continuous line) shows finite-size deviation. Wolff's single-cluster algorithm was used [14]. Each data set corresponds to average over $25,000,000$ independent realizations.

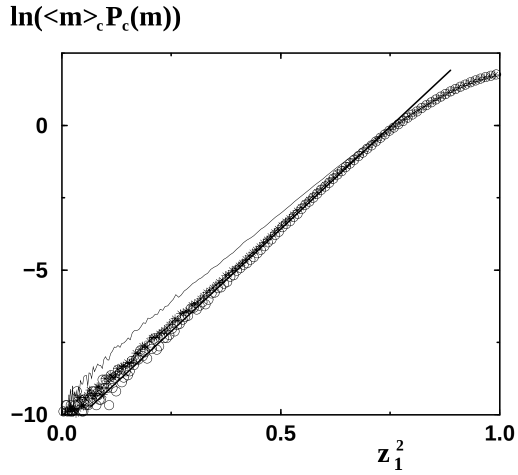

FIG. 2: Part $m \leq \langle m \rangle_c$ of the logarithm of the scaled PDF (4) *vs* z_1^2, for the 2D XY-model at $T = T_{BKT}$. The solid straight line is the best fit: $\ln(\langle m \rangle_c P_c(m)) = b_1 z_1^2$+cst for the $L = 128$, $z_1 < 0.8$, data. Numerically, $b_1 = 12.7$. Same symbols as in Fig.1.

[10]. In this region, $0 \leq T \leq T_{BKT}$, the system is critical, and asymptotic (*i.e.* $L \to \infty$) self-similarity results in the so-called first-scaling law [12]:

$$\langle m \rangle P(m) = \Phi_T(z_1) \qquad , \text{with} \quad z_1 \equiv \frac{m}{\langle m \rangle} , \qquad (4)$$

and Φ_T is a scaling function which depends only on the actual temperature T. Under this form, the hyperscaling relation, $\langle m \rangle / \sigma = cst$, is automatically realized. Eq.(4) is a sequel of the standard finite-size scaling theory [13], but it is highly advantageous that (4) does not require knowledge of any critical exponent. FIG.(1) gives numerical exemplification of the first-scaling law at T_{BKT}, and illustrates the overall shape of the distribution $\Phi_c(z_1)$ (hereafter, the index 'c' refers to the BKT critical point, $T = T_{BKT}$).

We separate the free energy $\mathcal{F}$ of the 2D XY-system at equilibrium (temperature $T = 1/\beta$) into the sum of a regular part describing the small values of the magnetization, a singular part [15] vanishing as the essential singularity [16, 17] when $T \to T_{BKT}$, and a regular part for the large values of the magnetization, namely:

$$\beta \mathcal{F}(m) = \varphi_0(m/\langle m \rangle) + \varphi_S(m/\langle m \rangle) + \varphi_\infty(m/\langle m \rangle) \ . \quad (5)$$

Clearly, discussion on the system behavior can be carried out either through the free energy (5) or the first-scaling law (4), since: $\ln P(m) = -\beta \mathcal{F}(m)$+constant term.

The regular small-m tail. – As the singular behavior should vanish at the BKT transition, we study first the regular small-m behavior of $P(m)$ at $T = T_{BKT}$. Numerical results for $P_c(m)$ are shown on FIG.2 in the form (4). They suggest the leading form:

$$\ln P_c(m) \approx b_1 \left(m / \langle m \rangle_c \right)^2 \ . \qquad (6)$$

Close to the most probable value of the magnetization, Eq.(2) and Eq.(6) are indeed consistent each other as the latter writes : $\ln P_c(m) = \text{cst} + 2 b_1 z_\sigma / (\langle m \rangle_c / \sigma_c) + \mathcal{O}(z_\sigma^2)$, in which we recognize the term linear in z_σ.

The singular small-m tail. – We consider now the singular part of the free energy through the combination:

$$\ln \left(\langle m \rangle P(m) \right) - \ln \left(\langle m \rangle_c P_c(m) \right) \qquad (7)$$

vs the reduced magnetization $z_1 \equiv m / \langle m \rangle$. The data plotted in FIG.3, suggest a cubic z_1^3-behavior:

$$\varphi_S(z_1) \approx c(T) z_1^3 \ , \qquad (8)$$

for every $T < T_{BKT}$, and for the values of m smaller than the mean. Moreover, $c(T_{BKT}) = 0$.

The large-m tail at the BKT point. – Instead of using multicanonical Monte-Carlo simulations [18] which need too large system sizes to conclude [19], we consider static in-plane magnetic field, $\mathbf{H}$, as a probe to study the features of the PDF for the large values of the magnetization. Indeed, as the intensity of $\mathbf{H}$ increases, the most probable magnetization, $m_H^\star$, as well as its mean value, $\langle m_H \rangle$, explores larger values of the PDF tail. We consider two alternative forms for the critical tail, namely:

• the 'Gumbel-like' shape (2) – noted below: ' hypothesis (G)' –, which writes in the first-scaling form:

$$\Phi_c(z_1) \sim \exp\left(-\lambda_0 e^{a_0 z_1}\right) \qquad \text{for} \qquad z_1 \to \infty \ , \qquad (G)$$

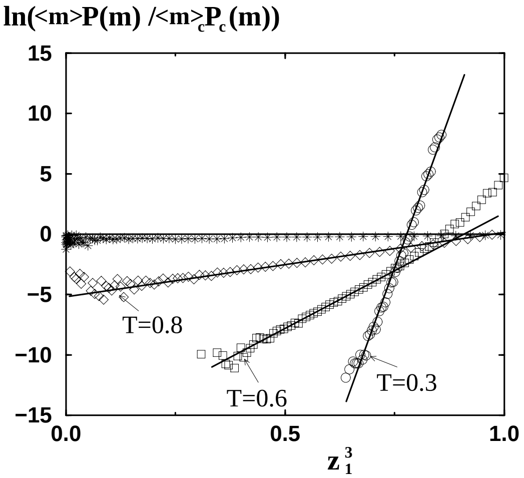

FIG. 3: Part $m \leq \langle m \rangle$ of the logarithm of the scaled PDF, corrected by the regular part of the free energy (see (7)), for $L = 16$ and four different temperatures: $T = 0.3$ (circles), $T = 0.6$ (squares), $T = 0.8$ (diamonds), and $T = 0.885$ (stars) which is close to the critical temperature ($T_{BKT} \approx 0.893$ [20]). The plot is versus $z_1^3 \equiv (m/\langle m \rangle)^3$. The straight lines are the best fits Eq.(8).

with $a_0 = a_\sigma \times (\langle m \rangle_c / \sigma_c)$ (≈ 16.4 from (3) and Table I), and $\lambda_0 = \lambda_\sigma e^{-a_0}$. It is the form suggested in [4, 5, 6];

• the 'Weibull-like' critical shape – noted below: ' hypothesis (W)' –, which is [21]:

$$\Phi_c(z_1) \sim \exp(-\lambda_1 z_1^{\delta+1}) \qquad \text{for} \qquad z_1 \to \infty \ , \qquad (W)$$

with λ_1 a positive parameter, and $\delta + 1 = 16$ [22].

Let ϕ be the direction of $\mathbf{H}$ with respect to the x-axis (*i.e.* $\mathbf{H} = (H\cos\phi, H\sin\phi)$). According to general thermodynamics, the magnetization PDF is given by: $P_c(m, H) \propto \exp(-\beta_c \mathcal{F} + \beta_c L^2 m H \cos(\psi - \phi))$, with the field-less free energy $\mathcal{F}$. Therefore, the most probable magnetization, $m_H^\star$, is the solution of the equation $\partial P_c(m, H)/\partial m = 0$ for a given value of H. As the instantaneous magnetization direction ψ should coincide with the magnetic field direction ϕ for the large systems, we use $\cos(\psi - \phi) \approx 1$. Rewritten in terms of the auxiliary variables $X \equiv H/\langle m \rangle_c^\delta$ and $Y \equiv H/m_H^{\star\delta}$, Eqs.(5),(6), with hypothesis (G) or (W), result respectively in:

$$\frac{X}{A} + 2b_1 \left(\frac{X}{Y}\right)^{1/\delta} = \lambda_0 a_0 \, e^{a_0 (X/Y)^{1/\delta}} \qquad (9)$$

or

$$= \lambda_1 (\delta + 1) \, \frac{X}{Y} \ , \qquad (10)$$

which are implicit equations for the most probable magnetization, $m_H^\star$, (written in the combination Y) vs the magnetic field H and the system size N (written in the combination X). The constant A is such that: $A^{-1} = \beta_c L^2 \langle m \rangle_c^{\delta+1} \approx 1.07$.

For the large magnetic field, $m_H^\star$ is expected to be much larger than $\langle m \rangle_c$, that is: $X/Y \gg 1$. Consequently, the solution of Eq.(9) is:

$$Y = a_0^\delta \, X/(\ln X + C)^\delta \qquad (11)$$

where $C = -\ln(A\lambda_0 a_0) \approx 14.2$ is a positive constant. Within the hypothesis (W), one has: $(X/Y)^{1/\delta} \ll X/Y$,

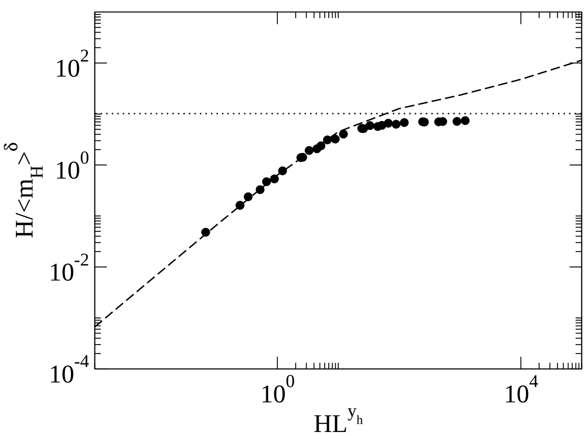

FIG. 4: Double-logarithmic plot of $H/\langle m_H \rangle^\delta$ *vs* the reduced magnetic field HL^{y_H} with: $y_H = 2\delta/(\delta+1)$. These two variables are convenient for the numerical simulations and simply related to the variables X and Y of the text: $H/\langle m_H \rangle^\delta = Y \times (m_H^\star/\langle m_H \rangle)^\delta$ and $HL^{y_H} = X \times (A\beta_c)^{-\delta/(\delta+1)}$, with the constant values: $(m_H^\star/\langle m_H \rangle)^\delta \approx 1$ and $(A\beta_c)^{-\delta/(\delta+1)} \approx 0.96$. The dashed curve is the solution of the first Eq.(9) (corresponding to the hypothesis (G)), while the dotted line is Eq.(12), with $\lambda_1 = \lambda_\sigma$ in agreement with (14). The system size goes from $L = 16$ up to $L = 512$. Each point corresponds to an average over 100,000 independent realizations [23].

such that (10) shows that Y is asymptotically a constant:

$$Y \approx A\lambda_1(\delta + 1) \ . \qquad (12)$$

So, increase of Y with the intense magnetic field should be interpretated as failure of (W).

Inference from the numerical simulations. – Both solutions, (11) and (12), are drawn on FIG.4 in comparison with the results of large-scale numerical simulations of the 2D XY-model with the in-plane magnetic field at the BKT temperature. It is clear that the numerical simulations are consistent with the hypothesis (W), while the double-exponential tail (G) should be discarded. This suggests the following form of the critical

TABLE I: Temperature, system size, average magnetization per spin, ratio of average magnetization to standard deviation. The best fit for the latter is: $\langle m\rangle_c/\sigma_c = 14.81 - 21.5/L$, at the BKT temperature, $T_{BKT} = 0.893$.

T	L	$\langle m\rangle$	$\langle m\rangle/\sigma$
0.3	16	0.923218	66.958
0.6	16	0.836307	29.249
0.8	16	0.764091	18.260
0.885	16	0.723259	13.907
0.893	16	0.718814	13.467
0.893	32	0.662819	14.119
0.893	64	0.611181	14.486
0.893	96	0.582217	14.583
0.893	128	0.563209	14.644
0.893	256	0.518921	14.687
0.893	512	0.478045	14.829

PDF for the 2D XY-model:

$$P_c(m) \propto e^{b_1 z_1^2 - \lambda_1 z_1^{16}} \quad , \quad z_1 \equiv m/\langle m\rangle \ . \qquad (13)$$

Below the BKT critical temperature, additional term $+c(T)z_1^3$ should appear in the exponential.

In order to understand the origin of the approximation (2), let us change the reduced magnetization according to: $z_1 = 1 + z_\sigma/(\langle m\rangle/\sigma)$. At T_{BKT}, and for the small values of $z_\sigma/(\langle m\rangle_c/\sigma_c)$ (recall that $\langle z_\sigma\rangle = 0$, and that $\langle m\rangle_c/\sigma_c \approx 14.8$ is a rather large number), we obtain:

$$P_c(m) \propto e^{2b_1 z_\sigma/(\langle m\rangle_c/\sigma_c) - \lambda_1(1+z_\sigma/(\langle m\rangle_c/\sigma_c))^{16}} \ .$$

Writing then $1 + z_\sigma/(\langle m\rangle_c/\sigma_c) \approx e^{z_\sigma/(\langle m\rangle_c/\sigma_c)}$, yields Eq.(2), provided the following relations are verified:

$$a_\sigma = \frac{16}{\langle m\rangle_c/\sigma_c} \quad ; \quad b_\sigma = \frac{2b_1}{\langle m\rangle_c/\sigma_c} \quad ; \quad \lambda_\sigma = \lambda_1 \ , \qquad (14)$$

So, Eq.(2) appears to be a good approximation around the most probable magnetization, but is inconsistent with the general critical relation $\langle m_H\rangle \propto H^{1/\delta}$, unlike Eq.(13). By the way, the conjectured relation [5] $b_\sigma/a_\sigma = \pi/2$ writes simply: $b_1 = 4\pi$, that we accept here as a new conjecture (numerically: $b_1 \approx 12.7$, see FIG.2).

Conclusion. – In this Letter, we explained how using the field conjugated to the order parameter provides unique information about the tail of the probability distribution function of the order parameter. This is of major importance for the critical systems, since the shape of the tail is directly linked to the value of a critical exponent. Therefore, this general method provides alternative way to calculate or measure the critical exponent δ.

We chose the critical 2D XY-model as a debated example to treat with this method. Indeed, a former double-exponential approximation of the magnetization PDF in the 0-magnetic field is found to be inconsistent with the critical behavior of the system - though correct near the most probable magnetization -. Moreover, this approximation being taken from another field of statistical physics, could mislead, as it suggests hidden link between these two fields. The new proposed approximation corrects these flaws.

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